

紫茎泽兰的化学成分初报

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关键词 紫茎泽兰; 正三十二烷; β -谷甾醇; 豆甾醇; 蒲公英醇棕榈酸酯; 蒲公英醇乙酸酯

紫茎泽兰 (*Eupatorium adenophorum* Spreng) 原产中美墨西哥, 现在滇南一带广泛分布, 对林、牧业生产造成严重危害。其化学成分研究未见报道。

从紫茎泽兰的叶和花序中, 分到九个单体, 经详细的光谱解析和与标准品对照, 其中五个成分的化学结构分别为: 正三十二烷 *n*-dotriacontane (1), β -谷甾醇 β -sitosterol (2), 豆甾醇 *stigmasterol* (3), 蒲公英醇棕榈酸酯 *taraxasteryl palmitate* (4), 蒲公英醇乙酸酯 *taraxasteryl acetate* (5)。

1. 正三十二烷 *n*-dotriacontane (1), $C_{32}H_{66}$, mp 48—49°C, IR (KBr): 2950, 2915, 2850, 1474, 1464, 1376, 730, 720 cm^{-1} . 1H NMR ($CDCl_3$) δ : 0.88 (3H, t, 6.5, 2 \times Me), 1.25 (br. s. 30 \times CH₂)。MS *m/z*: 409, 337, 323, 309, 295, 281, 267, 253, 239, 225, 211, 197, 183, 169, 155, ……71 (base peak)。与文献^[1]值一致。

2. β -谷甾醇 β -sitosterol (2), $C_{29}H_{50}O$, mp 110—112°C, 白色针晶。IR (KBr): 3410, 1655, 1640, 1050, 1018, 955, 834, 796 cm^{-1} . 1H NMR ($CDCl_3$): 0.68 (3H, s, 18-Me), 1.01 (3H, s, 19-Me), 0.84 (3H, d, 6.5, 21-Me), 0.74, 0.91 (each 3H, d, 7.0, 26-, 27-Me), 0.85 (3H, t, 6.5, 29-Me), 1.65 (1H, s, OH), 3.58 (1H, m, $W_{\frac{1}{2}} = 22Hz$, 3 α -H), 5.35 (1H, d, 4.7, 6-H)。MS *m/z*: 414 (M^+), 396, 381, 367, 351, 329, 303, 273, 255, 241, 231, 213, 199, 185, ……55 (base peak)。与文献^[1, 4]值一致。

3. 豆甾醇 *stigmasterol* (3), $C_{29}H_{48}O$, mp 141—142°C, 白色针晶。IR (KBr): 3350, 1660, 1636, 1045, 1015, 963, 952, 830, 790, 768, 712 cm^{-1} . 1H NMR ($CDCl_3$) δ : 0.70 (3H, s, 18-Me), 1.01 (3H, s, 19-Me), 1.22 (3H, d, 6.5, 21-Me), 0.79, 1.02 (each 3H, d, 6.5, 26-, 27-Me), 0.87 (3H, t, 7.0, 29-Me), 1.25 (1H, s, OH), 3.58 (1H, m, $W_{\frac{1}{2}} = 22Hz$, 3 α -H), 5.08 (2H, t, 5.6, 22-, 23-H), 5.35 (1H, d, 5.9, 6-H)。MS *m/z*: 412 (M^+),

399, 369, 351, 329, 314, 300, 271, 255, 229, 213, 199, 176,55 (base peak). 与文献值^[1, 3, 4]一致。

4. 蒲公英醇棕榈酸酯 taraxasteryl palmitate (4), $C_{46}H_{80}O_2$, mp 93—94 °C, 白色针晶。

其红外光谱中最特征的是中等强度间隔约为 21 cm^{-1} 的一组峰: 1341, 1320, 1299, 1278, 1255, 1235, 1213, 1186, 1162 cm^{-1} 这是长链脂肪酸及其酯的特征吸收带。此外, 该成分还呈现酯的特征强吸收峰: 1722 cm^{-1} , 环外末端双键吸收: 1633 cm^{-1} , 以及角甲基和异丙基引起的吸收: $1382, 1375\text{ cm}^{-1}$ 。 $^1\text{H NMR}$ (CDCl_3) δ : 0.85, 0.85, 0.85, 0.88, 0.93, 1.02 (each 3H, s, $6 \times \text{Me}$), 1.02 (3H, d, 6.5, 29-Me), 0.85 (3H, t, 7.0, Me- CH_2), 1.25 (br. s, 26H, $13 \times \text{CH}_2$), 2.17 (1H, quintet, 6.5, 19-H), 2.30 (2H, t, 7.0, $-\text{CH}_2-\text{COO}$), 4.50 (1H, dd, 10, 6, $3\alpha\text{-H}$), 4.61 (2H, d, 2, 30- H_2), 0.65—2.30 (24H, methylene and methines). MS m/z : 664 (M^+), 621, 581, 564, 551, 508, 482, 410, 409, 257, 189,69 (base peak). 与文献^[2-4]值一致。

5. 蒲公英醇乙酸酯 taraxasteryl acetate (5), $C_{32}H_{52}O_2$, mp 238—240 °C, 白色片状晶。

(5) 的 $^1\text{H NMR}$ 谱与 (4) 的差异仅仅在于: 在 $\delta\ 2.04\text{ ppm}$ 处多了一个乙酰氧基信号, 少了链状亚甲基引起的 $\delta\ 1.25\text{ ppm}$ 强吸收。

IR (KBr): 1723, 1636, 1383, 1370, 1360, 1238, 1084, 1015, 1005, 973, 963, 890, 865, 818 cm^{-1} 。 $^1\text{H NMR}$ (CDCl_3) δ : 0.85, 0.85, 0.85, 0.89, 0.89, 0.97 (each 3H, s, $6 \times \text{Me}$), 0.93 (3H, d, 6.5, 29-Me), 2.04 (3H, s, OAc), 4.48 (1H, dd, 10, 6, $3\alpha\text{-H}$), 4.71 (2H, d, 4, 30- H_2), 0.70—2.30 (25H, methylene and methines). MS m/z : 468 (M^+), 408, 299, 249, 229, 219, 218, 204, 189,43 (base peak)。以上数据与文献^[2, 4]报道值相吻合。

熔点用 Kofler 显微测熔仪测定, 未校正。红外光谱用 Shimadzu IR-450 型仪测定。核磁共振谱用 Bruker WH-90 PFT 脉冲付立叶变换波谱仪测定, 以 TMS 为内标, δ (ppm) 表示化学位移。

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A BRIEF REPORT OF THE CHEMICAL CONSTITUENTS FROM EUPATORIUM ADENOPHORUM

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Abstract We examined the chloroform extract of the leaves and inflorescence of *Eupatorium adenophorum* Spreng collected in the suburb of Kunming, Yunnan, China. Nine colourless crystals were isolated. Five among them were identified to be dotriacontane (1), β -sitosterol (2), stigmasterol (3), taraxasteryl palmitate (4), taraxasteryl acetate (5) by spectroscopic evidences and comparison with standard samples.

Key words *Eupatorium adenophorum*, Dotriacontane, β -sitosterol, Stigmasterol, Taraxasteryl palmitate, Taraxasteryl acetate